



chain nodes :

21 22 23 24 25 26 27 28 29 30 31 37

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

chain bonds :

2-12 3-22 4-21 5-23 9-25 16-26 23-24 25-26 25-27

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 7-12 8-9 8-14 9-10 10-11 12-13 13-14 15-16
15-20 16-17 17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 2-3 2-12 3-4 3-22 4-5 4-21 7-12 8-14 9-25 12-13 13-14

exact bonds :

5-23 16-26 23-24 25-26 25-27

normalized bonds :

6-7 6-11 7-8 8-9 9-10 10-11 15-16 15-20 16-17 17-18 18-19 19-20

G1:Br,F,I,COOH,CN,SO2,SO3H,CHO,NO2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
31:CLASS 32:Atom 33:Atom 34:Atom 35:Atom 37:CLASS 38:Atom